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Dear Bolko,

This is the second quarterly report of our third year in the Thin Film Partnership Program (Subcontract No. XXL-5-44205-12 to University of Nevada, Las Vegas: Characterization of the electronic and chemical structure at thin film solar cell interfaces). A brief summary and details of our activities are given below. This report is in fulfillment of the deliverable schedule of the subcontract statement of work (SOW).

Summary

This project is devoted to deriving the electronic structure of interfaces in $Cu(In,Ga)(S,Se)_2$ and CdTe thin film solar cells. By using a unique combination of spectroscopic methods (photoelectron spectroscopy, inverse photoemission, and X-ray absorption and emission) a comprehensive picture of the electronic (i.e., band alignment in the valence and conduction band) as well as chemical structure is painted. The work focuses on (a) deriving the bench mark picture for world-record cells, (b) analyzing state-of-the-art cells from industrial processes, and (c) aiding in the troubleshooting of cells with sub-standard performance.

Surprisingly, very little is known about the chemical and electronic structure in *real-world industrial-grade* samples, i.e., manufactured in large-scale, high-throughput equipment in an industrial environment. Global Solar Energy, Inc. ("GSE"), e.g., has pioneered a unique robust process to manufacture CIGSe solar cell devices which can hardly be simulated on laboratory scale. While other companies pursue the approach of in-line deposition on rigid glass substrates, GSE is the only company to date using a roll-to-roll coating of the complete solar cell thin film layer stack on flexible substrates. Central questions of the latter approach are how the chemical structure of the deposited materials differs from that of conventionally prepared materials and how the process-specific parameters influence the material properties. The roll-to-roll process itself presents a set of process-specific challenges as well, such as chemical interactions between the deposited material (front side) and the back side of the flexible substrate during roll-up after each preparation step.

In order to shed light on these questions we have used x-ray photoelectron spectroscopy (XPS) and x-ray excited Auger electron spectroscopy (XAES) to investigate the chemical surface structure of selected samples (both, front and back sides) directly taken out of GSE's production process after each preparation step. Upon CIGSe formation preliminary data evaluation shows that the back side exhibits $MoSe_2$ and absorber related XPS and XAES features. Compared to the front side, we find an increased

amount of Ga on the back side which suggests a pronounced interaction with the front side upon roll-up.

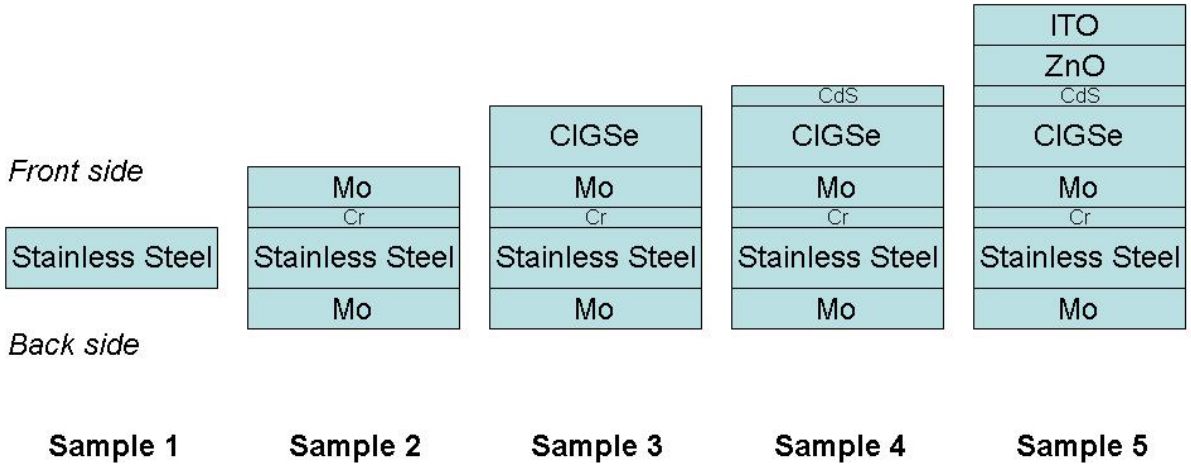

Fig. 1 *Schemes of the investigated samples.*

Detailed Description of the Activities:

In order to investigate the material properties in CIGSe-based thin film solar cells induced by roll-to-roll deposition on flexible substrates a set of samples directly taken out of the production process of Global Solar Energy, Inc. ("GSE") was investigated. For the different samples which represent the status after individual deposition steps in the manufacturing process, both, the front and back side was investigated by x-ray photoelectron spectroscopy (XPS) and x-ray excited Auger electron spectroscopy (XAES).

Fig. 1 shows respective schemes of the investigated test structures. Shown is a typical structure used by GSE for their commercial PV process. Different materials are being utilized at GSE for the top electrode. In this specific case ZnO and ITO was used.

Fig. 2 shows the survey spectra of the front (top panel) and back side (bottom panel) of the investigated test structures. For the front side samples we find the elements of the respective deposited material. As indicated by the small C 1s (and O 1s) XPS peak the surface contamination could successfully be minimized due to a suitable packaging and shipping procedure. We find a relatively high amount of oxygen on sample #2, which points to the formation of MoO_x. The back side samples (except #1) are dominated by Mo-related XPS signals. Surprisingly, we find a relatively high amount of selenium for samples #3 - #5 which is indicative for the formation of $MoSe_2$ upon absorber formation (see also detail spectra in Fig. 4). Furthermore, we find CIGSe-related XPS peaks on back side sample #3 and #4 (see also the detail spectra in Fig. 3), which are explained by an interaction of front side absorber material with the back side during roll-up of the stainless steel tape after CIGSe deposition.

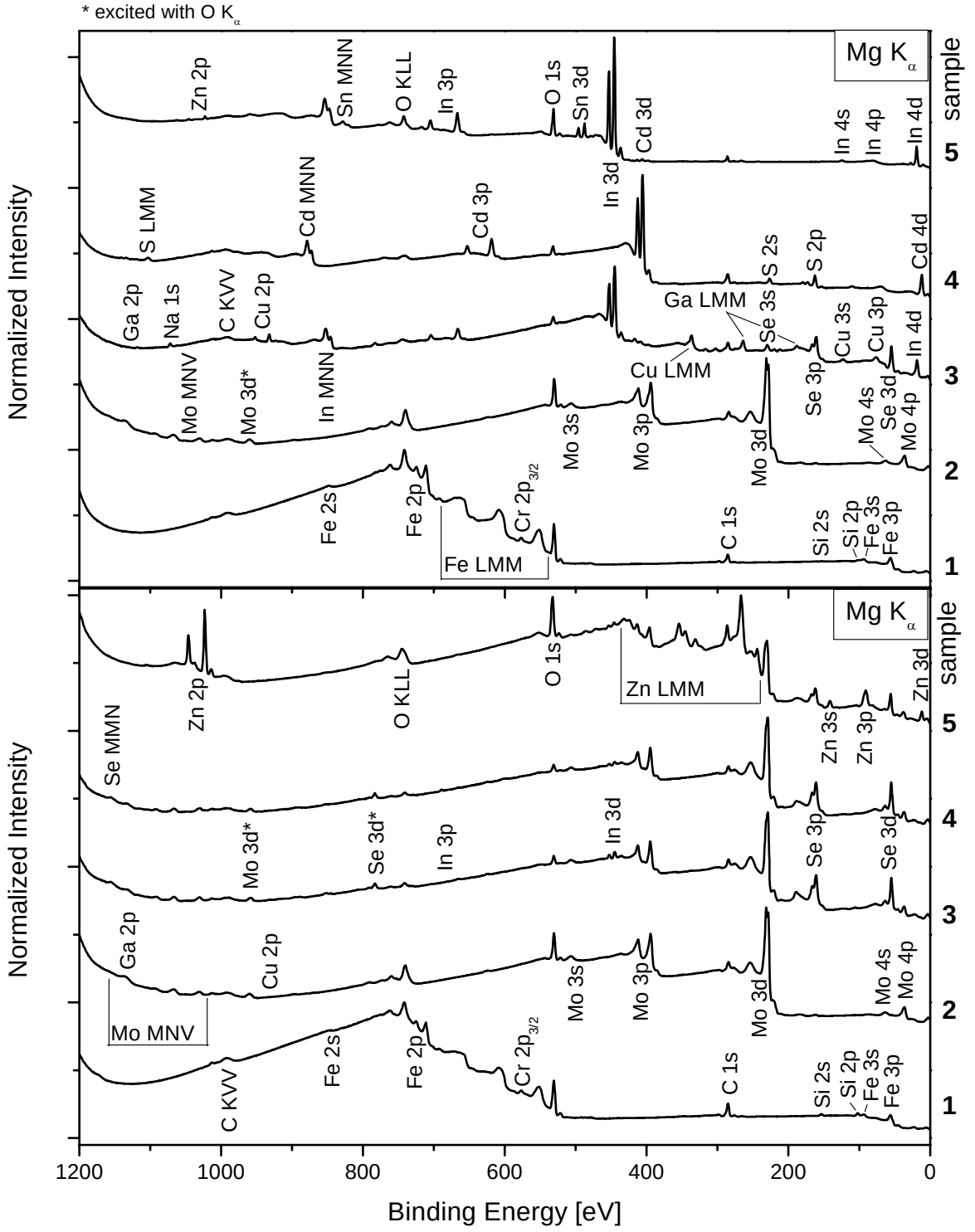

Fig. 2 *XPS survey spectra of the front (top panel) and back side (bottom panel) of the investigated test structures.*

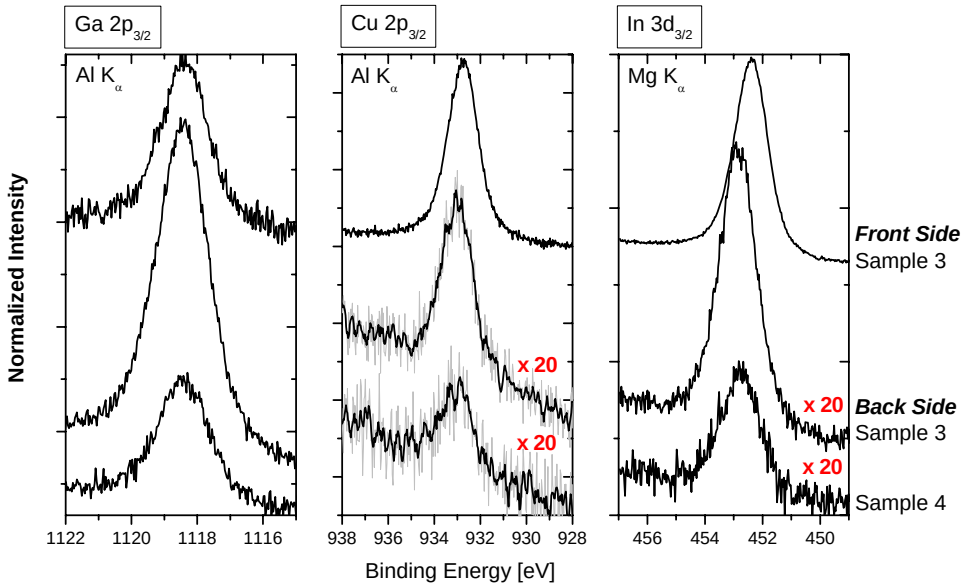

Fig. 3 *XPS Ga $2p_{3/2}$ (left), Cu $2p_{3/2}$ (center), and In $3d_{3/2}$ (right) detail spectra of the front side sample #3 (top spectra) and the back side samples #3 and #4 (bottom two spectra).*

The comparison of the Ga $2p_{3/2}$, Cu $2p_{3/2}$, and In $3d_{3/2}$ detail spectra of the front side sample #3 and the back side samples #3 and #4 in Fig. 3 shows an abundance of Ga at the back side sample surfaces (note the magnification factors indicated for the Cu $2p_{3/2}$ and In $3d_{3/2}$ XPS peaks of the back side samples). This can be interpreted not only as a simple deposition of front side material on the back side, but indicates a significant chemical interaction leading to the observed Ga accumulation.

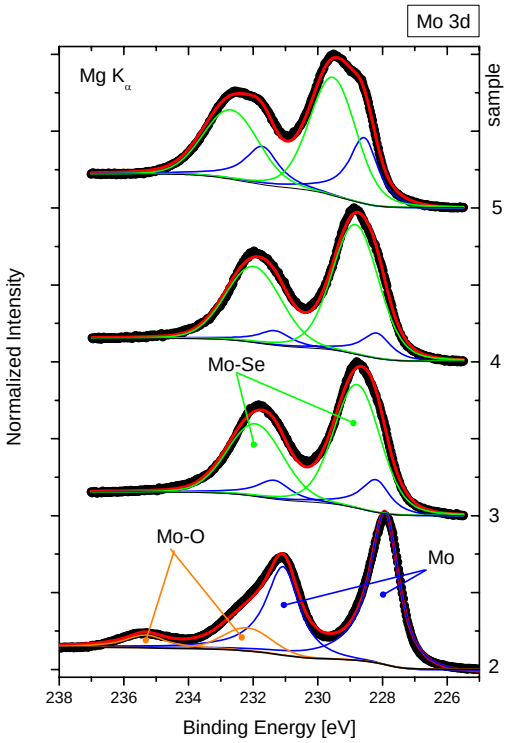

Fig. 4 *XPS Mo 3d detail spectra of the back side samples #2-5 (experimental data shown as dots, fits indicated by solid lines).*

Fig. 4 shows the XPS Mo 3d detail spectra of the back side samples #2-5. For all spectra, we find pronounced spectral features which deviate from a Mo 3d spectrum of a single Mo species. By peak fitting the spectra of sample #1, we were able to identify two Mo 3d doublets which we ascribe to metallic Mo and Mo-O bonds, respectively. As indicated by the pronounced change in the spectral shape of the Mo 3d spectra after CIGSe deposition (sample #3) and confirmed by our peak fit analysis, the (oxidized) Mo is converted into $MoSe_2$ upon absorber formation. The fact that the metallic Mo 3d doublet is still visible indicates that the $MoSe_2$ layer might not be closed or too thin (i.e., thinner than the XPS information depth) to completely attenuate the Mo 3d photoelectrons stemming from the underlying metallic Mo.

In a next step, it is planned to investigate the impact of the absorber forming high temperature preparation step (where the stainless steel substrate is held at a temperature above 500°C) on the diffusion/intermixing characteristic of the Mo/stainless steel interface.

If you have any questions, please do not hesitate to call me at (702) 895-2694.

Sincerely,

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